

Up and Down Quark Masses and Corrections to Dashen's Theorem from Lattice QCD and Quenched QED

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In a previous Letter [Borsanyi *et al.*, Phys. Rev. Lett. **111**, 252001 (2013)] we determined the isospin mass splittings of the baryon octet from a lattice calculation based on $N_f = 2 + 1$ QCD simulations to which QED effects have been added in a partially quenched setup. Using the same data we determine here the corrections to Dashen's theorem and the individual up and down quark masses. Our ensembles include 5 lattice spacings down to 0.054 fm, lattice sizes up to 6 fm, and average up-down quark masses all the way down to their physical value. For the parameter which quantifies violations to Dashen's theorem, we obtain $\varepsilon = 0.73(2)(5)(17)$, where the first error is statistical, the second is systematic, and the third is an estimate of the QED quenching error. For the light quark masses we obtain, $m_u = 2.27(6)(5)(4)$ and $m_d = 4.67(6)(5)(4)$ MeV in the modified minimal subtraction scheme at 2 GeV and the isospin breaking ratios $m_u/m_d = 0.485(11)(8)(14)$, $R = 38.2(1.1)(0.8)(1.4)$, and $Q = 23.4(0.4)(0.3)(0.4)$. Our results exclude the $m_u = 0$ solution to the strong CP problem by more than 24 standard deviations.

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The up (u) and down (d) quark masses are two fundamental parameters of the standard model of particle physics. These masses cannot be directly determined through experiment because of the confinement of quarks within hadrons. Lattice QCD provides an *ab initio* approach to the non-perturbative calculation of QCD correlation functions. This method can be used to determine the light quark masses from the experimental values of hadron masses. While it has become relatively straightforward to determine the isospin averaged mass m_{ud} of the up and down quarks in pure QCD (see Refs. [1] for a recent review), a direct determination of the individual masses of the up and down quarks is a significantly more challenging task [2]. A large part of the difficulties arises from the need to include QED, a theory without a mass gap, into finite-volume lattice calculations.

The inclusion of QED effects in lattice QCD calculations was pioneered almost 20 years ago using a quenched approximation in which both strong and electromagnetic sea-quark effects are neglected [3]. Since then many determinations of the light-quark mass difference, $\delta m = m_u - m_d$ have appeared that rely on phenomenological estimates of EM corrections [2,4–6]. Direct inclusion of quenched QED effects was first picked up again in Ref. [7] for $N_f = 2$, and in Ref. [8] for $N_f = 2 + 1$. More recent calculations can be

found in Refs. [9–12]. See Ref. [1] for further details. In this Letter we present a determination of δm by including quenched QED effects atop $N_f = 2 + 1$ QCD configurations that were previously used for an *ab initio* determination of m_{ud} [5,6]. Such a setup is necessarily partially quenched, because valence and sea quark masses renormalize differently, as discussed below. Our ensembles include pion masses at or below the physical point as well as five different lattice spacings and multiple large volumes so that systematic errors of the continuum and finite volume extrapolations can reliably be estimated. This is a sequel to the Letter [13] which uses the same data set to compute light octet baryon isospin mass splittings. Note that a calculation of octet baryon and other hadron mass isospin splittings in unquenched QCD + QED, with pion masses down to 195 MeV, can be found in Ref. [14]. Here, because we are dealing with light quark masses whose extraction requires reaching deep into the chiral regime [15], we favor the data set used in Ref. [13]. It also has the notable advantage that the s and average u - d quark masses have been determined [5,6]. Thus, all of the relevant nonperturbative renormalization and running has already been performed in pure QCD [6].

The light-quark mass difference δm is connected, through a low-energy theorem [16], to the pseudoscalar

meson EM mass splittings. In the late 1960s, Dashen showed that pions and kaons receive the same EM contributions in the $SU(3)$ chiral limit [17]. This result is commonly known as *Dashen's theorem*. During the 1990s, attempts to compute the chiral corrections to Dashen's theorem in effective field theories led to controversial and surprisingly large results (cf. the review Ref. [18] for more details). In this Letter we present a computation of these corrections from our lattice QCD and quenched QED simulations.

General strategy.—To compute the quark mass difference δm , one must tune the parameters ($\alpha_s, \alpha, m_u, m_d, m_s$) of the theory so that the calculations of five, well-chosen observables reproduce their measured values. We define the physical point through the charged pion mass $M_{\pi^+}^2$, the combination $(M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)/2$, the kaon mass splitting $\Delta M_K^2 = M_{K^+}^2 - M_{K^0}^2$ and the electromagnetic coupling α set to its Thomson limit value [19]. The lattice spacings are determined using the isospin averaged Ξ mass or the Ω^- mass.

In this work we only consider the leading $O(\alpha, \delta m)$ corrections to isospin symmetry. We can therefore use as a proxy for δm the partially quenched quantity ΔM^2 , which is defined as the difference of the squared masses of the “connected” $\bar{u}u$ and $\bar{d}d$ pseudoscalar mesons [13]. Using ΔM^2 instead of δm we can circumvent the problem of determining explicitly the electromagnetic renormalization of the light quark masses which, due to our use of Wilson type fermions, has a continuum divergent additive component. It is known from partially quenched chiral perturbation theory coupled to photons (PQ χ PT + QED) [20] that ΔM^2 is related to δm by the following expansion:

$$\Delta M^2 = 2B_2\delta m + O(m_{ud}\alpha, m_{ud}\delta m, \alpha^2, \alpha\delta m, \delta m^2), \quad (1)$$

where B_2 is the two-flavor chiral condensate parameter. If the quark masses have their physical values, we can safely make the assumption that $O(m_{ud}) = O(\delta m)$. Then at the level of precision considered here, ΔM^2 is proportional to δm . It is therefore possible to extract δm from the physical value of ΔM^2 and the constant B_2 .

B_2 was recently computed in Ref. [15], using the same QCD simulations as the ones considered in the present Letter. In this Letter we compute the physical value of ΔM^2 by considering the leading isospin expansion of the kaon mass splitting ΔM_K^2 :

$$\Delta M_K^2 = C_K\alpha + D_K\Delta M^2. \quad (2)$$

Results for ΔM_K^2 obtained for different values of α and δm from lattice QCD and QED simulations can be fitted to this expression to obtain the coefficients C_K and D_K and, subsequently, the value of ΔM^2 corresponding to physical quark masses, from the experimental value of ΔM_K^2 .

Summary of the lattice methodology.—The lattice setup used for this project is very similar to Ref. [13] and is based on our set of lattice QCD simulations presented in Ref. [6]. It is composed of 47 $N_f = 2 + 1$ QCD ensembles with pion masses down to 120 MeV, 5 lattice spacings down to 0.054 fm, and 16 different volumes up to $(6 \text{ fm})^3$. These simulations were performed using a tree-level $O(a)$ -improved Wilson fermion action with 2 steps of HEX smearing. For each QCD configuration, a QED one is generated using the noncompact Maxwell action in Coulomb gauge with the four-momentum zero mode fixed to 0. The resulting $SU(3) \times U(1)$ configuration is then included in the Wilson-Dirac operator used to compute the valence-quark propagators, with the appropriate electric charge. For each ensemble, two sets of valence-quark propagators were typically produced with the physical value of the electric charge. For the first set, the bare PCAC masses of the light and strange quarks are tuned to the values of the sea quarks without QED, thus eliminating the α/a divergent renormalization of the bare quark masses. For the second set we keep m_s and m_u fixed to their values in the first set, but varied m_d to allow ΔM^2 , and thus δm , to bracket its physical value. On one particular QCD ensemble, we perform three valence analyses: two with close to physical δm and a value of α either about twice or one-fourth its physical value, and a third with $\alpha \approx 0$ and $\delta m \approx 0$. A plot of the values of M_{dd}^2 versus M_{uu}^2 used in our valence data sets can be found in Ref. [13] (Fig. 1).

In this setup, two approximations are made: the sea u and d quark masses have the same mass and they carry no electric charge (QED is quenched). It is straightforward to show that the splitting of the sea light-quark masses only affects isospin splittings at orders in the isospin expansion which are beyond those considered. Regarding the

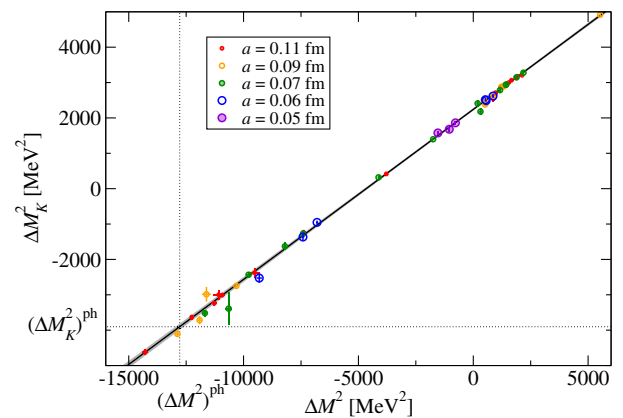


FIG. 1. Example of a fit of the dependence of ΔM_K^2 on α and ΔM^2 to the expression of Eq. (2). Here, ΔM_K^2 is plotted as a function of ΔM^2 . The dependence of the lattice results on all other variables has been subtracted using the fit. The fit has a correlated χ^2/dof equal to $61.57/45 = 1.37$, corresponding to a p value of 5%. It is plotted as a solid curve, with its 1σ band.

quenching of QED, large N_c counting and $SU(3)$ flavor symmetry suggests that the sea QED effects may represent $O(10\%)$ of the $O(\alpha)$ contribution to a given isospin splitting [13]. Considering the EM part of the kaon splitting, which is of particular interest here, the next-to-leading order (NLO) $PQ\chi PT + QED$ calculation of Ref. [20] can be used to estimate the QED quenching effects. In Ref. [21] we argue that they may represent 5% of the $O(\alpha)$ correction. Nevertheless, for giving the reader an idea of how such a quenching uncertainty may propagate to the other quantities studied in this Letter, we retain the more conservative 10% quenching uncertainty on $\Delta_{QED}M_K^2 = \alpha C_K$.

The EM contribution to the kaon splitting.—In the expansion (2), the coefficients C_K and D_K still depend on m_{ud} , m_s , a , and the temporal and spatial extents T and L . We fix m_{ud} and m_s to their physical values by matching to the experimental values of $M_{\pi^+}^2$ and the combination $(M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)/2$. Then, as explained in detail in Ref. [13], we use as a model for ΔM_K^2 a first order expansion of C_K and D_K in these mass parameters around the physical mass point. Additionally, we allow for $O(a)$ discretization effects and powerlike $O(1/L)$ finite-volume effects [14,22] in the QED contribution proportional to C_K , as required in our setup. The finite volume effects are taken into account by adding the following term to the aforementioned expansion of C_K :

$$C_K^{FV} = -\frac{\kappa M_K}{L} \left[1 + \frac{2}{M_K L} \left(1 - \frac{\pi T}{2\kappa L} \right) \right] + \frac{\rho}{L^3}, \quad (3)$$

where $\kappa = 2.837\dots$ is a known number, $M_K = \frac{1}{2}(M_{K^+} + M_{K^0})$ is the isospin averaged kaon mass and ρ is a fit parameter. In the parametrization (3), the $O(1/L)$ and $O(1/L^2)$ coefficients have been fixed to their known universal value [14] and the $O(1/L^3)$ term is fitted to take into account additional structure-dependent effects. For the QCD contribution proportional to D_K , we assume $O(\alpha_s a, a^2)$ discretization effects and negligible finite-volume effects, which is justified in our large volumes given our present precision. To estimate systematic uncertainties, we consider a variety of analysis procedures. These variations are identical to those performed in Ref. [13]. They include (please see Ref. [13] for justifications and additional details) fitting the needed correlators on a conservative or a more aggressive time range, setting the scale with the mass of the Ω^- or the isospin-averaged Ξ ; eliminating points with M_{π^+} either greater than 400 or than 450 MeV for the Ω^- and the Ξ mass, and greater than 350 or than 400 MeV for ΔM_K^2 , and including either $\alpha_s a$ or a^2 contributions in D_K ; replacing individually the Taylor mass expansions in C_K and D_K by the inverse of these expansions (for a total of 4 choices). This leads to 128 different determinations of C_K and D_K . An example of such a fit is illustrated in Figs 1–3. Finally, using the histogram method developed in Ref. [23], we combine all of these results to obtain

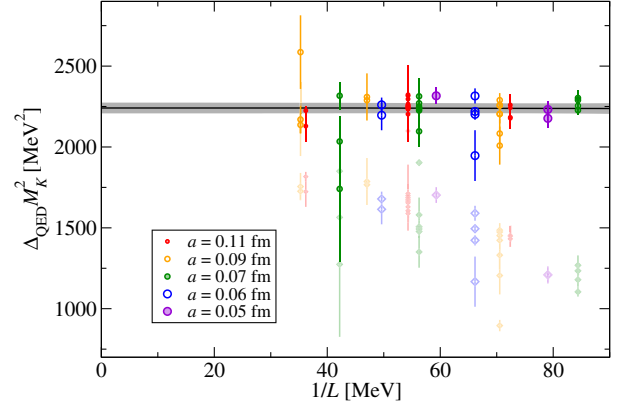


FIG. 2. Same fit as in Fig. 1. Here $\Delta_{QED}M_K^2$ is plotted as a function of $1/L$. The gray symbols show the full volume dependence of the data. For the plain symbols, the universal $O(1/L)$ and $O(1/L^2)$ finite volume effects from Eq. (3) have been subtracted and the fit to the $O(1/L^3)$ correction is plotted.

$$\Delta_{QED}M_K^2 = 2186(26)(68)(219) \text{ MeV}^2, \quad (4)$$

where C_K is taken at the physical mass point, in the continuum and infinite volume limits. Here, and in the following equations, the first error is statistical, the second is systematic, and the third is an estimation of the quenching uncertainty as discussed above. Our result can be compared to an estimate obtained from the input of FLAG [1], $\Delta_{QED}M_K^2 = 2090(380) \text{ MeV}^2$, which is based on phenomenologic and early lattice determinations. The results are entirely compatible and ours has a total precision which is more than 5 times higher omitting the generous estimate for the quenching error and more than 1.6 times including it. For completeness, we also give the value of the slope of ΔM_K^2 in ΔM^2 at the physical point, obtained from our analysis: $D_K = 0.484(5)(4)$. This result is compatible with the value $D_K = 0.45(9)$, obtained by appropriately combining results from FLAG [1]. Its total error is 15 times more precise.

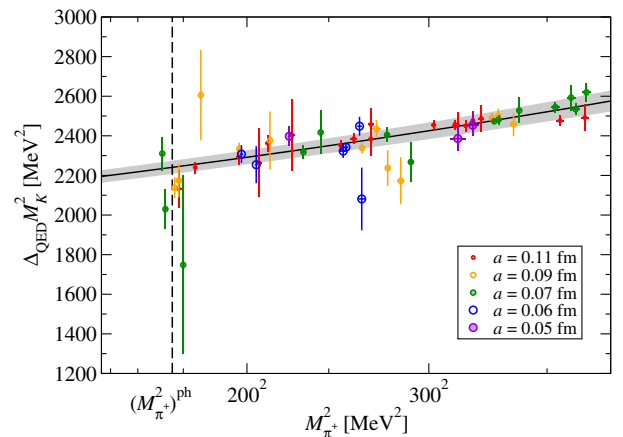


FIG. 3. Same fit as in Fig. 1. Here $\Delta_{QED}M_K^2$ is plotted as a function of $M_{\pi^+}^2$.

Corrections to Dashen's theorem.—As defined in Ref. [1], one can quantify corrections to Dashen's theorem with the parameter

$$\varepsilon = \frac{\Delta_{\text{QED}} M_K^2 - \Delta_{\text{QED}} M_\pi^2}{\Delta M_\pi^2}. \quad (5)$$

The pion isospin mass splitting, needed to evaluate ε , is challenging to obtain through a lattice computation. Because the neutral pion is diagonal in flavor, correlation functions for this state will contain quark disconnected diagrams. These diagrams are known to be expensive and hard to evaluate on the lattice. Thus, we choose not to compute the pion splitting here. Fortunately, using G parity, one can easily show that the leading $O(\delta m)$ corrections to ΔM_π^2 vanish. Therefore, at the level of precision considered in this Letter, we have $\Delta_{\text{QED}} M_\pi^2 = \Delta M_\pi^2$, which is very well known experimentally [24].

Using our result (4) for $\Delta_{\text{QED}} M_K^2$ and the experimental value of ΔM_π^2 , we obtain

$$\varepsilon = 0.73(2)(5)(17). \quad (6)$$

Now, if we include an estimate of the δm^2 corrections in the relation of $\Delta_{\text{QED}} M_\pi^2$ to ΔM_π^2 , as given in Ref. [1] with the parameter $\varepsilon_m = \Delta_{\text{QCD}} M_\pi^2 / \Delta M_\pi^2 = 0.04(2)$, we find $\varepsilon = 0.77(2)(5)(17)(2)$, with the fourth uncertainty due to ε_m . Our result of Eq. (6) can be compared to the FLAG estimate $\varepsilon = 0.7(3)$ [1].

Up and down quark masses.—Using our analysis of the kaon splitting, the experimental value of this splitting, our lattice result $B_2 = 2.61(6)(1)$ GeV [15] in the modified minimal subtraction ($\overline{\text{MS}}$) scheme at 2 GeV and formula (2), we obtain

$$\delta m = m_u - m_d = -2.41(6)(4)(9) \text{ MeV} \quad (7)$$

in the same scheme and at the same scale. It is interesting to note that the quenching of QED has a rather small impact on the determination of δm . This comes essentially from the fact that the QCD part of the kaon splitting is roughly 3 times larger than the QED part. Our result is entirely compatible with the value $\delta m = -2.53(16)$ MeV, derived from FLAG input [1].

If we combine Eq. (7) with our previous result $m_{ud} = 3.469(47)(48)$ MeV [5], we get

$$m_u = m_{ud} + \frac{\delta m}{2} = 2.27(6)(5)(4) \text{ MeV}, \quad (8)$$

$$m_d = m_{ud} - \frac{\delta m}{2} = 4.67(6)(5)(4) \text{ MeV}, \quad (9)$$

still in the $\overline{\text{MS}}$ scheme at 2 GeV. Again, our results are nicely compatible with the FLAG [1] values $m_u = 2.16(9)(7)$ and $m_d = 4.68(14)(7)$ MeV. From the results of Eqs. (8) and (9), we obtain the ratio of light quark masses

$$\frac{m_u}{m_d} = 0.485(11)(8)(14). \quad (10)$$

Strictly speaking, because u and d have different electric charges, this ratio is scale dependent in QCD plus QED. However, it is easy to see that this dependency is beyond the leading isospin order considered in this work. Our result is compatible with the FLAG estimate $m_u/m_d = 0.46(2)(2)$ [1].

We can further use our previous result $m_s/m_{ud} = 27.53(20)(8)$ [5] to build the flavor breaking ratios R and Q :

$$R = \frac{m_s - m_{ud}}{m_d - m_u} = 38.2(1.1)(0.8)(1.4), \quad (11)$$

$$Q = \sqrt{\frac{m_s^2 - m_{ud}^2}{m_d^2 - m_u^2}} = 23.4(0.4)(0.3)(0.4). \quad (12)$$

These results are compatible with the FLAG estimates $R = 35.0(1.9)(1.8)$ and $Q = 22.5(6)(6)$ [1]. It is interesting to compare our results for R to those obtained from χ PT applied to $\eta \rightarrow 3\pi$ decays [16,25–28]. The convergence of χ PT for this process is very poor and it is usually supplemented by a dispersive analysis. Without such an analysis, the results vary from 19.1 at LO to 31.8 at NLO and 42.2 [or 38.7 setting the $O(p^6)$ low-energy constants to 0] at NNLO [25]. The most recent NNLO χ PT dispersive analysis [27] gives $R = 37.7(2.2)$, in good agreement with our result.

To summarize, our results are compatible with the estimates of Ref. [1], which already include input from the quenched QED studies mentioned above [29]. In most cases, they significantly improve on their precision. In all isospin symmetry breaking quantities the quenching uncertainty is the dominant one. Therefore, it is now important to determine these quantities using a fully unquenched calculation with significantly higher statistics similar to what was done for the splitting of stable hadrons in Ref. [14].

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